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# Semi-empirical analysis of the fine structure and oscillator strengths for atomic strontium

J. Ruczkowski [a,*], M. Elantkowska [b], J. Dembczyński [a]

[a] Institute of Control and Information Engineering, Faculty of Electrical Engineering, Poznań University of Technology, Piotrowo 3A, 60-965 Poznań, Poland
[b] Laboratory of Quantum Engineering and Metrology, Faculty of Technical Physics, Poznań University of Technology, Piotrowo 3, 60-965 Poznań, Poland

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ABSTRACT

As the result of our studies on the atomic structure of complex atoms we produced high quality wave functions for both even and odd systems of configurations of Sr I. These wave functions were used for the parametrization of the oscillator strengths for electric-dipole transitions, where reliable data were available. The angular coefficients of the transition matrix in pure *SL* coupling were calculated by means of straightforward Racah algebra. The transition matrix was transformed into the actual intermediate coupling by the fine structure wave functions. The transition integrals were treated as free parameters in the least squares fit to the *gf* values. This procedure allowed us to obtain the values of the transition integrals and predict the values of oscillator strengths for the transitions from odd levels in a wide spectral range.



## 1. Introduction

Accurate oscillator strengths (*gf*-values) are among the most important kinds of atomic data. They are of particular importance in astronomy, for reliable determinations of chemical abundances in stellar atmospheres, in plasma physics, and for comparison with theoretical works.

Recently, we developed a semi-empirical method for determining oscillator strengths that is an alternative to the commonly used, purely theoretical calculations, or to the semi-empirical approach combined with theoretically calculated transition integrals [1]. The angular coefficients of the transition matrix in pure *SL* coupling were calculated from straightforward Racah algebra. The transition matrix was transformed into the actual intermediate coupling by the fine structure eigenvectors obtained using a semi-empirical method. The transition integrals were treated as free parameters in the least squares fit to experimental *gf* values. As an example, the results of the calculation for the electric dipole transitions for Sc II were presented. In the subsequent papers this method was applied for titanium, niobium and vanadium ions [2–4]. Recently, the calculation results for hafnium and zirconium ions obtained using this method were compared with the results of a pseudo-relativistic Hartree–Fock calculations including core polarization effects [5,6].

In the present paper, we describe the electric-dipole transitions in neutral strontium. The main motivation for this study is a direct determination of the radial integrals for the transitions from the levels belonging to Rydberg series, with principal quantum number up to $n=20$.

Strontium is a member of the alkaline earth group of elements. There are four stable and one unstable isotopes of strontium. The emission spectrum of neutral strontium has been studied since the early 1900s [7–12]. The measurements of the strontium spectra in the range of 2300–10 036 Å were published by Sullivan in 1938 [13]. These results, along with the unpublished material of

* Corresponding author. Tel.: +48 616653228; fax: +48 616652563.
*E-mail address:* jaroslaw.ruczkowski@put.poznan.pl (J. Ruczkowski).

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**Table 1**
Values of the intraconfiguration fine structure parameters ($cm^{-1}$).

| Parameter | Value | | HFR |
|---|---|---|---|
| *Even configurations* | | | |
| $E_{AV}(4d^2)$ | 40 684 | (54) | 41 107 |
| $F^2(4d,4d)$ | 15 867 | (*) | 15 867 |
| $F^4(4d,4d)$ | 9740 | (*) | 9740 |
| $\zeta(4d)$ | 62 | (14) | 66 |
| $D^0(n_0d4d,4d4d)\zeta(n_0d,4d)$ | 24 | (17) | |
| $E_{AV}(4d\ 5s)$ | 17 557 | (16) | 20 121 |
| $G^2(4d,5s)$ | 10 720 | (140) | 14 312 |
| $D^0(n_0d5s,4d5s)\zeta(n_0d,4d)$ | −24 | (8) | |
| $D^0(n_0d5s,4d5s)D^0(n_0d5s,4d5s)$ | −440 | (60) | |
| $E_{AV}(4d\ 5d)$ | 46 888 | (31) | 50 754 |
| $F^2(4d,5d)$ | 2859 | (78) | 3245 |
| $F^4(4d,5d)$ | 2360 | (110) | 1738 |
| $G^0(4d,5d)$ | 5020 | (150) | 4790 |
| $G^2(4d,5d)$ | 3340 | (130) | 2492 |
| $G^4(4d,5d)$ | 2953 | (160) | 1611 |
| $\zeta(5d)$ | 11 | (*) | 11 |
| $D^0(n_0d5d,4d5d)\zeta(n_0d,4d)$ | 36 | (11) | |
| $E_{AV}(4d\ 6d)$ | 53 019 | (24) | 54 838 |
| $E_{AV}(4d\ 7d)$ | 57 339 | (23) | 56 804 |
| $E_{AV}(4d\ 8d)$ | 58 191 | (16) | 57 917 |
| $E_{AV}(4d\ 9d)$ | 58 817 | (16) | 58 606 |
| $E_{AV}(4d\ 10d)$ | 59 181 | (12) | 59 062 |
| $E_{AV}(4d\ 5g)$ | 56 230 | (11) | 56 214 |
| $F^2(4d,5g)$ | 127 | (32) | 181 |
| $F^4(4d,5g)$ | 15 | (*) | 15 |
| $G^2(4d,5g)$ | 2 | (*) | 2 |
| $E_{AV}(5s^2)$ | 3333 | (35) | 3333[a] |
| $E_{AV}(5s\ 6s)$ | 29 780 | (27) | 29 933 |
| $G^0(5s,6s)$ | 1186 | (67) | 932 |
| $E_{AV}(5s\ 5d)$ | 33 017 | (19) | 35 867 |
| $G^2(5s,5d)$ | 478 | (120) | 1309 |
| $E^0(n_0d5s,5d5s)E^0(n_0d5s,5d5s)$ | −370 | (*) | |
| $D^0(n_0d5d,5s5d)D^0(n_0d5d,5s5d)$ | 700 | (*) | |
| $E_{AV}(5s\ 5g)$ | 41 543 | (*) | 41 916 |
| $E_{AV}(5p^2)$ | 40 954 | (77) | 38 877 |
| $F^2(5p,5p)$ | 16 420 | (460) | 14 840 |
| $\zeta(5p)$ | 191 | (36) | 255 |
| $D^0(n_0p5p,5p5p)\zeta(n_0p,5p)$ | −2590 | (420) | |
| $E_{AV}(5p\ 6p)$ | 55 157 | (23) | 57 478 |
| $F^2(5p,6p)$ | 815 | (87) | 3412 |
| $G^0(5p,6p)$ | 1782 | (22) | 1236 |
| $G^2(5p,6p)$ | 741 | (15) | 1144 |
| $E^0(n_0p6p,6p5p)\zeta(n_0p,5p)$ | −107 | (24) | |
| $E_{AV}(4f^2)$ | 100 065 | (*) | 95 401 |
| $F^2(4f,4f)$ | 7274 | (*) | 7274 |
| $F^4(4f,4f)$ | 4740 | (*) | 4740 |
| $F^6(4f,4f)$ | 3466 | (*) | 3466 |
| $E_{AV}(4f\ 5p)$ | 74 223 | (*) | 62 318 |
| $F^2(4f,5p)$ | 1928 | (*) | 1928 |
| $G^2(4f,5p)$ | 524 | (*) | 524 |
| $G^4(4f,5p)$ | 346 | (*) | 346 |
| *Odd configurations* | | | |
| $E_{AV}(4d\ 5p)$ | 38 253 | (37) | 35 173 |
| $F^2(4d,5p)$ | 8444 | (42) | 10 127 |
| $G^1(4d,5p)$ | 12 791 | (78) | 8860 |
| $G^3(4d,5p)$ | 3418 | (36) | 5713 |
| $\zeta(4d)$ | 111 | (3) | 112 |
| $\zeta(5p)$ | 263 | (23) | 159 |
| $D^2(4dn_0p,4d5p)\zeta(n_0p,5p)$ | 161 | (32) | |
| $D^0(n_0d5p,4d5p)E^1(n_0d5p,5p4d)$ | −916 | (154) | |
| $E_{AV}(4d\ 6p)$ | 49 878 | (21) | 49 749 |
| $E_{AV}(4d\ 7p)$ | 55 122 | (28) | 54 413 |
| $E_{AV}(4d\ 8p)$ | 56 785 | (22) | 56 590 |
| $E_{AV}(4d\ 9p)$ | 57 914 | (11) | 57 792 |
| $E_{AV}(4d\ 4f)$ | 53 299 | (16) | 53 475 |
| $F^2(4d,4f)$ | 760 | (*) | 600 |
| $F^4(4d,4f)$ | 220 | (*) | 167 |
| $G^1(4d,4f)$ | 1346 | (112) | 116 |
| $G^3(4d,4f)$ | 68 | (*) | 68 |
| $G^5(4d,4f)$ | 47 | (*) | 47 |
| $E_{AV}(5s\ 5p)$ | 18 205 | (49) | 16 483 |
| $G^1(5s,5p)$ | 14 386 | (38) | 17 947 |
| $E_{AV}(5s\ 6p)$ | 34 660 | (59) | 34 743 |
| $E_{AV}(5s\ 4f)$ | 39 095 | (39) | 39 142 |
| $G^3(5s,4f)$ | 151 | (23) | 138 |

* Denotes an fixed parameter.
[a] Denotes arbitrarily assumed value of the center of gravity of the configuration.

**Table 2**
Values of selected configuration interactions radial parameters ($cm^{-1}$). The complete table is presented in supplementary material.

| Configurations | Parameter | Value | | HFR |
|---|---|---|---|---|
| *Even configurations* | | | | |
| $4d^2 \leftrightarrow 4d5s$ | $R^2(4d4d,4d5s)$ | −22 110 | (260) | −14 158 |
| $4d^2 \leftrightarrow 4d5d$ | $R^0(4d4d,4d5d)$ | 951 | (*) | 951 |
| | $R^2(4d4d,4d5d)$ | 5321 | (*) | 5321 |
| | $R^4(4d4d,4d5d)$ | 3470 | (*) | 3470 |
| $4d^2 \leftrightarrow 4d5g$ | $R^2(4d4d,4d5g)$ | −191 | (*) | −191 |
| | $R^4(4d4d,4d5g)$ | −81 | (*) | −81 |
| $4d^2 \leftrightarrow 5s^2$ | $R^2(4d4d,5s5s)$ | 16 980 | (180) | 14 491 |
| $4d^2 \leftrightarrow 5s6s$ | $R^2(4d4d,5s6s)$ | 1164 | (92) | 1198 |
| $4d^2 \leftrightarrow 5s5d$ | $R^2(4d4d,5s5d)$ | −4335 | (79) | −3362 |
| $4d^2 \leftrightarrow 5s5g$ | $R^2(4d4d,5s5g)$ | 239 | (*) | 239 |
| $4d^2 \leftrightarrow 5p^2$ | $R^1(4d4d,5p5p)$ | 15 106 | (42) | 14 577 |
| | $R^3(4d4d,5p5p)$ | 11 104 | (67) | 9118 |
| *Odd configurations* | | | | |
| $4d5p \leftrightarrow 4d6p$ | $D^0(4d5p,4d6p)$ | 3000 | (*) | 0 |
| | $D^2(4d5p,4d6p)$ | 3610 | (160) | 3494 |
| | $E^1(4d5p,6p4d)$ | 3201 | (*) | 3201 |
| | $E^3(4d5p,6p4d)$ | 2232 | (*) | 2232 |
| $4d5p \leftrightarrow 4d4f$ | $D^2(4d5p,4d4f)$ | −1514 | (*) | −1514 |
| | $D^4(4d5p,4d4f)$ | −665 | (*) | −665 |
| | $E^1(4d5p,4f4d)$ | −1087 | (*) | −1087 |
| | $E^3(4d5p,4f4d)$ | −603 | (*) | −603 |
| $4d5p \leftrightarrow 5s5p$ | $D^2(4d5p,5s5p)$ | −11 090 | (260) | −11 406 |
| | $E^1(4d5p,5p5s)$ | −11 280 | (200) | −12 490 |
| $4d5p \leftrightarrow 5s4f$ | $D^2(4d5p,5s4f)$ | 2340 | (140) | 1835 |
| | $E^1(4d5p,4f5s)$ | 1571 | (*) | 1571 |

* Denotes a fixed parameter.

Humphreys and Russell, were used by Moore to develop the comprehensive table of strontium energy levels [14]. In 2010, a detailed overview of the research papers concerning wavelengths, energy levels and transition probabilities for atomic strontium, was presented by Sansonetti and Nave [15]. Their paper contained a critical review of the spectroscopic data for neutral strontium, such as the energy levels with designations and uncertainties, wavelengths with classifications, intensities and transition probabilities, which were tabulated.

Recently, Civiš et al. reported the study of the Sr I infrared spectra in the range of 1300–5000 $cm^{-1}$ using high-resolution Fourier spectroscopy [16]. They determined the previously unknown excitation energies of the 5g, 6g and 6h states and also calculated a large list of transition probabilities and oscillator strengths in the observed spectral range, using the quantum defect theory.